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EQUATIONS OF A SIMPLE FLAME SOLVED BY SUCCESSIVE APPROXIMATIONS TO THE SOLUTION OF AN INTEGRAL EQUATION*

(PART II: SECOND ORDER REACTION)

G. Klein

ABSTRACT

The problem of an idealized flame whose underlying chemical reaction is unimolecular and reversible (where the kinetic energy of the gas stream is neglected), which has been solved by an integral equation method of successive approximations for a first reaction in PART I, is now extended to a second order reaction. This problem is very nearly equivalent to that of a simple chain reaction flame in which the catalyst reaction(s) are assumed to be in equilibrium. In this case the behavior near the hot boundary of the functions involved is very different from that of the case of a first order reaction, and a careful choice of the integral equation and of the lowest approximation to be adopted has to be made. -The diffusion coefficient is assumed constant: for a certain value of this constant the problem simplifies considerably and for other values of an alternative perturbation and expansion method is proposed which involves only linear differential equations. - It is verified that neglect of the back reaction affects the method and results immaterially, and the effect of varying of hot boundary temperature is briefly considered.

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EQUATIONS OF A SIMPLE FLAME SOLVED BY SUCCESSIVE APPROXIMATIONS TO THE SOLUTION OF AN INTEGRAL EQUATION

Series 8
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by G. Klein

which will be referred to as

(PART I: FIRST ORDER REACTION)

REFERENCES

1) J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, Molecular Theory of Gases and Liquids. Wiley, (1954). Chapter 11.7.

2) C. F. Curtiss, J. O. Hirschfelder, and D. E. Campbell, The Theory of Flame Propagation and Detonation, III, University of Wisconsin Naval Research Laboratory Report, 15 Feb. 1952 (where a detailed numerical solution of the problem is given in the appendix); Reprinted without appendix in 4th Int. Symp. for Combustion, p. 190, Publ. by Williams and Wilkins (1953).

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1. INTRODUCTION

The problem of an idealized flame whose underlying chemical reaction is unimolecular, reversible, and of the first order, which has already been treated and solved in the references quoted below, is reconsidered here (kinetic energy of the gas stream being neglected). Its solution is made to depend on the solution of an integral equation which contains an unknown parameter whose eigenvalue has to be determined. This equation is solve by a method of successive approximations.

Except for minor and obvious deviations, * the notation is the same as that used in the first reference quoted; equations there are referred to on the left margin.

(11.7-27)
$$\frac{d}{dt} = \frac{d}{dc}$$
 (-eliminating the distance variable)

(11.7-25)
$$R(x, \tau) = -f(x, \tau)$$
 (-an essentially positive quantity)

(11.7-31)
$$\mathcal{E} = \frac{1}{1-y} \frac{i}{\beta}$$
 (-for conciseness)

^{*} The only ones being (cf. equations 1.1-1.3)

2

Flame equations. These are, in terms of demensionless variables and parameters, the equations of continuity (for chemical reaction), diffusion, and energy (or thermal conduction),

(11.7-25)
$$q \frac{dG}{d\tau} = \frac{1}{\mu^2} R(1,\tau)$$
 1.1

(11.7-28)
$$G \frac{dx}{dz} = \frac{1}{\delta} (x - G)$$
(11.7-31
$$G = \frac{1}{b} (G G_{\infty}) - (z_{\infty} - z)$$
1.3

Hot Boundary conditio is. At the hot boundary chemical reaction, diffusion and thermal conjuction cease. Thus

(11.7-32)
$$R(x_{\infty}, k_{\infty}) = 0$$
 , 1.4
(11.7-34) $x_{\infty} = G_{\infty}$ 1.5

$$(11.7.34) / x_{\infty} = G_{\infty} 1.5$$

Equation 1.3, is the integrated energy balance equation, and by suitable choice of the constant of integration the third boundary condition, that the temperature gradient must vanish,

$$g(\bar{c}_{\infty})=0$$

has already been taken care of.

Cold boundary conditions. If one assumes a conventional functional ass ive two avaction tens, where the latter does not actually vanish at the cold boundary temperature, some care is needed in the stipulation of the cold boundary conditions. Experimentally, however, and in computanon where in any case one contines oneself to a limited number of decimal places, the reaction rate can be taken as zero at and near the cold boundary temperature. Thus in practice there is no doubt what the conditions should be, they are analogous to those at the hot boundary, wiz,

$$R(x_{\alpha}, \tau_{\alpha}) = 0$$

(11.7-35)
$$x_0 = G_0 = 1$$

$$q(z_s) = 0 1.9$$

Auxiliary quantities. It is convenient to define the known linear

$$x'' = x_{\infty} + b(r_{\infty} - \tau)$$
 1.10

and the parameter $q = \frac{1}{b\mu^2}$ 1.11

3

Elimination of the mass rate of flow. We consider the temperature gradient and the concentration as the primary dependent variables.

From 1.3, 1.5, and 1.10,

so that if the temperature gradient is known, the fractional mass rate of flow. G. can be readily found.

Fundamental simultaneous equations. With 1.12, 1.10 equations 1.1, 1.2 may be written in the form

$$q\left(1-\frac{dq}{d\tau}\right) = q R(x,\tau)$$

$$= x^* + \left(b \div b \frac{dx}{d\tau}\right) q$$
1.13

These equations have to be satisfied simultaneously, the solu' one being embject to the boundary conditions. It should be noted that this is an eigenvalue problem; the pavameter q in 1.13 is not known and depends on the boundary conditions.

Special cases. In the following two cases the problem simplifies considerably:

When dai . it is clear from 1.10 that 1.14 is satisfied by

$$X_{\delta^{*}i} = X^{*}$$
, 1.15

and hence the problem reduces to the solution of the single differential equation

$$q_{\delta=1}\left(1-\frac{dq_{\delta-1}}{dz}\right)=q_{\delta-1}R(x^*,z)$$
 1.16

When &= 0, equation 1.14 gives

(11.7-44)
$$x_{5=0} = x^{2} + bq_{5=0}$$
 1.17

which when substituted into 1.13 again leads to a single differential equation.

$$q_{\delta=0} \left(1 - \frac{dq_{\delta>0}}{dt} \right) = q_{\delta=0} R \left(x^* + bq_{\delta=0}, t \right)$$
1.18

This latter equation simplifies further if the reaction rate is linear in the fuel gas concentration.

EQUATIONS OF A SIMPLE FLAME SOLVED BY SUCCESSIVE APPROXIMATIONS TO THE SOLUTION OF AN INTEGRAL EQUATION

Semiers 8 WIS-ONR-B 9 June 1954

(PART 1: FIRST ORDER REACTION)

List of Errata:

On cover and title page add: (PART I: FIRST ORDER REACTION)

- P. 1, first equation in the foetnote should read; $g \frac{d}{dx} = \frac{d}{d\xi}$
- P. 7. last symbol in equation 2.4 should be T.
- P. 7. first factor on the right of equation 2.5 should be $(\tau_a \tau_b)$
- P. 7, in the line before eqs. 2.8 the reference should be to eqs. 1.21
- P. 9, graph 4: the point $q_{(a)} = 398.5$ should have been marked

LIST OF SYMBOLS (in the order in which they occur)

7. REVISION: Fundamental simultaneous differential equations; Boundary conditions: Auxiliary functions; Summary ond-the hop-boundary

In the simple flame problem considered in PART I we have adopted τ the reduced temperature as independent variable and the temperature gradient as the main dependent variable: these two are related to the reduced distance 5

$$q = \frac{d\tau}{d\zeta} .$$

It has been shown (cf. 1.13, 1.14, 1.10) that the problem of a simple unimolecular flame is contained in the equations

$$q\left(1-\frac{dq}{d\tau}\right) = q R(x,\tau)$$
 7.2

$$(1.14) \qquad \qquad \chi - \chi^* \qquad = \qquad \left\{ (1-\delta)^{\frac{1}{2}} + \delta \frac{d(\overline{\chi} - \chi^*)}{d\tau} \right\} q \qquad 7.3$$

together with the boundary conditions

$$\chi(\tau_{\infty}) = \chi_{\infty} , \quad q(\tau_{\infty}) = 0 , \quad 7.4$$

$$(1.4) R(x_{\omega}, \tau_{\omega}) = 0 , 7.5$$

where it is assumed that the total reaction rate $R(x, \tau)$ for practical purposes vanishes at and near the cold boundary To.

×* in 7.3 is linear in The function and coincides with X at the boundaries, thus the fuel component

$$\frac{x^* - x_{\infty}}{x_0 - x_{\infty}} = \frac{\overline{t_{\infty}} - \overline{t}}{\overline{t_{\infty}} - \overline{t_{0}}}.$$

 $\mathcal{E} = \frac{x_0 - x_{\infty}}{t_{\infty} - t_{\alpha}}$ 7.8

and previously we had written (cf. 1.10)

Also,

$$\chi^* = \chi_{\infty} + \ell(\tau_{\infty} - \tau) . \qquad 7.9$$

It will be useful to define a fictitious beyond-the-hot-boundary temperature $\tau_{\infty}^{\#} > \tau_{\infty}$, where

so that 7.7 may be written more concisely as

$$\chi^* = \mathcal{C}(\tau_\infty^* - \tau)$$
 by the solution beside 7.11

and we note

$$\chi^{*}(\tau_{*}) = \chi_{*}$$
 $\chi^{*}(\tau_{*}) = \chi_{*}$ 7.12

It has already been remarked (cf. 1.15), and it is easily verified by inspection of the equation, that in the case $\delta = /$ a solution of 7.3 is $x = x^{2}$; in this case the right hand member of 7.2 does not contain f: the function f: f: wholly known. This, and the form of equation 7.3 suggest adopting the new variable

$$\xi = x - x^*, \qquad 7.14$$

replacing X, and expanding

$$R(x,t) = \mathcal{R}_{*}(t) + \mathcal{R}_{*}(t)(x-x^{*}) + \mathcal{R}_{*}(t)(x-x^{*})^{2} + \cdots 7.15$$

Here

$$\mathcal{R}_{s}(\tau) = R(x^{*}, \tau)$$
 7.16

and the other functions $\mathcal{R}_{1}(\tau)$, $\mathcal{R}_{2}(\tau)$, . . . , are similarly known if the form of the reaction rate is given. We write

$$R(x,\tau) = \mathcal{R}(\xi,\tau)$$
. 7.17

Cf. grapt 11.

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Summary. In terms of the functions just defined we have

$$\mathcal{R}(\xi,\tau) = \mathcal{R}(t) + \mathcal{R}(\tau)\xi + \mathcal{R}(t)\xi^2 + \dots, \quad 7.18$$

and the fundamental equations 7.1-7.3 may be written

$$q\left(i - \frac{dq}{d\tau}\right) = q \mathcal{R}(\xi, \tau)$$

$$\frac{d\xi}{d\tau} = \frac{ij}{q}$$

$$\frac{d\xi}{d\tau} - \frac{1}{q} \xi = -(1 - \xi) \xi$$
7.19
7.20

The boundary conditions 7.4-7,6 have now, in view of 7.14. 7.12, the simple form

$$\mathcal{E}(\tau_{\infty}) = 0 \qquad ; \qquad q(\tau_{\infty}) = 0 \qquad 7.22$$

$$\mathcal{E}(\tau_{\infty}) = 0 \qquad , \qquad q(\tau_{\infty}) = 0 \qquad 7.23$$

$$\mathcal{E}(\tau_{\infty}) = 0 \qquad , \qquad q(\tau_{\infty}) = 0 \qquad , \qquad 7.24$$

and it is understood that for practical purposes the functions $\mathcal{R}_{s}(r)$, $\mathcal{R}_{s}(r)$, $\mathcal{R}_{s}(r)$, $\mathcal{R}_{s}(r)$, vanish at and near the cold boundary \overline{c}_{s} .

Alternative summary in which 7.20, 7.21 are written in integrated form;

$$\frac{g\left(1-\frac{dq}{d\tau}\right)}{\xi} = \frac{g\left(\xi,\tau\right)}{\xi}; \quad g\left(\xi,\tau\right) = 0, \quad g\left(\xi_{\omega}\right) = 0$$

$$\xi = \int_{\frac{1}{2}}^{\frac{1}{2}} d\tau \quad 7.26$$

$$\xi = \frac{1-\delta}{\delta} \, \hat{\tau} \, e^{\frac{1}{3} \, \frac{\xi}{\delta}} \int_{\tau}^{\xi_{\omega}} e^{-\frac{1}{3} \, \frac{\xi}{\delta}} d\tau$$

$$7.27$$

and it is understood that the $\mathcal{R}_{\mathcal{L}}$ (τ), which are known functions, for practical purposes vanish at and near the cold boundary τ_o .

8. REACTION RATE AND NATURE OF THE SOLUTION

First order reaction. When the reaction is of the first order,

$$\mathcal{R}(\xi, t) = \mathcal{R}(\tau) + \mathcal{R}(\tau) \xi$$

This case has been dealt with in Part I where

$$(1.21) \qquad \mathcal{R}_{,}(z) = \psi(z)$$

 $\mathcal{R}_{\bullet}(z) = \mathcal{R}(z^{*}, z)$.
The total reaction rate $\mathcal{R}(\xi, z)$ has the single zero at $\mathcal{T}_{\bullet \bullet}$ where R. (T.) = 0 .

Second order reaction. Here

We shall consider the special case where the presence of the fuel is essential for both the forward and the back reaction: the fuel acts at the same time as a catalyst. Thus (cf. 7,14-7,17)

$$R(0,\tau) = 0$$
, i.e. $R(-x^*,\tau) = 0$. 8.2

Hence, by 7.15, or 8.1.

$$\mathcal{R}_{0}(\tau) = \chi^{**} \left\{ \mathcal{R}_{1}(\tau) - \chi^{**} \mathcal{R}_{2}(\tau) \right\}$$
 8.3
This implies that $\mathcal{R}_{0}(\tau)$ has two zeros, one at τ_{∞} , by 7.23,

and the other, due to the first factor on the right of 8.3 (cf. 7.11)

$$\mathcal{R}_{\mu}(\tau_{\mu}^{*})=0.$$

By 7.12 and 8.4,

$$X_{no} = \frac{\mathcal{R}_{n}(x_{no})}{\mathcal{R}_{n}(x_{no})}$$
8.6

The full reaction rate $R(\xi, \tau)$ will also, in general, have two serps, one at T. , and another beyond but near to T. ; in the case d=/.

cf. APPENDIX, p. 40

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Nature of the solution. The nature of the required solution for any given δ (where δ is of order unity) does not differ drastically from that of the case $\delta = /$, so that we confine ourselves to a short discussion of the latter. We have

$$q(1-\frac{dq}{dz}) = qR_{\rho}(z)$$
8.7

$$\mathcal{R}_{o}(\tau_{\bullet}) = 0$$
, $\left[\frac{d}{d\tau} \mathcal{R}_{o}(\tau)\right]_{T_{o}} = 0$; $\mathcal{R}_{o}(\tau) > 0$, $\tau_{\bullet} < \tau < \tau_{o}$; 8.8

$$\mathcal{R}_{o}(\tau_{\infty}) = 0, \quad \mathcal{R}_{o}(\tau_{\infty}^{*}) = 0, \quad 8.9$$

and the required solution must satisfy

$$a_{1}(\tau_{0}) = 0, \qquad g_{1}(\tau_{\infty}) = 0$$
8.10

The tangent elements of the family of integral curves of 8.7 are easily plotted from the relation

$$\frac{dq}{d\tau} = 1 - \frac{qR_0}{q}$$
8.11

The locus of stationary points of the integral curves is evidently the curve $q^{\mathcal{H}_0}(\tau)$; the τ -axis is the locus of points at which there is infinite slope; and the lines $\tau = \tau_{\infty}$, $\tau = \tau_{\infty}^*$, are loci of points at which there is gradient unity. There are two singular points, viz. on the τ -axis at $\tau = \tau_{\infty}$ and at $\tau = \tau_{\infty}^*$. The former is a saddle point and the required solution is the singular integral which passes through it with negative slope.

The parameter q in 8.7 is not known: instead there are two boundary conditions 8.10, i.e., q is an eigenvalue parameter. The nature of the second singular point at τ_{∞}^{*} depends on the magnitude of q - in the numerical application considered it is a spiral point (See graph 12.)

Series expansion near T_{∞} . Since $q(T_{\infty}) = 0$, $R_{\infty}(T_{\omega}) = 0$, one

finds easily from 8.7
$$\begin{bmatrix}
\frac{dq}{d\tau} \\
-\frac{d}{d\tau}
\end{bmatrix}_{\tau_o} = \frac{1}{2} \left\{ \sqrt{4q \left[-\frac{dR_o}{d\tau} \right]_{\tau_o}} + 1 - 1 \right\}$$

$$\begin{bmatrix}
\frac{d^2q}{d\tau^2} \\
-\frac{d^2}{d\tau^2}
\end{bmatrix}_{\tau_o} = q \begin{bmatrix}
\frac{d^2R_o}{d\tau^2} \\
-\frac{d^2}{d\tau^2}
\end{bmatrix}_{\tau_o} / \left(1 + 3 \left[-\frac{dq}{d\tau} \right]_{\tau_o} \right), 8.13$$
etc. from which a series expansion near τ_o may be obtained.

Solution near & in polar coordinates. Near & we put

$$q \mathcal{R}_{s}(\tau) = q \left[\frac{d \mathcal{R}_{o}}{d\tau} \right]_{\tau_{oo}} (\tau - \tau_{oo}) = m (\tau - \tau_{oo}), \quad 8.14$$

so that equation 8.7 becomes

$$\frac{dq}{d\tau} = \frac{q - m(\tau - \tau_e^*)}{q}$$
8.15

On changing to polar coordinates

$$q = r \sin \theta$$

$$\overline{\tau} - \overline{t} = r \cos \theta$$

$$8.16$$

$$8.17$$

and writing

$$t = \tan \theta$$
 8.18

one obtains the solution near τ_{∞}^* in the form

$$\Gamma = \Gamma_{-\frac{\pi}{2}} \left(\frac{t^{2} + 1}{t^{2} - t + m} \right)^{\frac{1}{2}} e^{\frac{t}{2} (m - \frac{t}{2})^{-\frac{1}{2}} \left(-\frac{\pi}{2} - tan^{-\frac{t}{2} - \frac{t}{2}} \right)} = \frac{t - \frac{t}{2}}{8.19}$$

That is, it is a spiral provided

$$49\left[\frac{dR.}{d\tau}\right]_{\tau_{co}^*} > 0$$
8.20

The nature of 9-(7) beyond 500 is of course of no physical interest.

9. INTEGRAL EQUATIONS AND METHOD OF SUCCESSIVE APPROXIMATIONS

In order to solve equations 7.25-7.27 we employ a method of successive approximations as follows. Suppose a ν -th approximation, $q^{(\nu)}$, to q is known: then by 7.26 and 7.27 we find the corresponding approximations to ξ and ξ thus:

$$\zeta^{(3)} = \int \frac{\tau_1}{g^{(3)}} d\tau \qquad 9.1$$

$$\xi^{(3)} = \frac{1-\delta}{\delta} \mathcal{E} e^{\frac{1}{\delta} \xi^{(3)}} \int_{e^{-\frac{1}{\delta}}}^{t_0} \xi^{(3)} d\tau \qquad 9.2$$

Equation 7.25 is the hard core of the problem. It is turned into an integral equation - but this can be done in an infinite number of ways: for instance, multiplication of 7.25 by 9^N , where N is not necessarily an integer, and integration, result in

$$\frac{1}{N+2}q^{N+2} = 9 \int_{\xi}^{\tau_{\infty}} q^{N} \mathcal{R}(\xi,\tau) d\tau - \int_{\xi}^{q^{N+1}} d\tau \cdot 9.3$$

One could now multiply 9.3 by some suitable function of N and add similar equations for all integers N starting from N=0; and would thus obtain an integral equation in well-known analytic functions of g. However, we have not succeeded in determining which functions would be the most 'natural' ones to take, and therefore confine ourselves to an integral equation of the form 9.3 for a suitable N.

In 9.3 the upper boundary condition has been taken care of; the lower boundary condition fixes the value of the eigenvalue parameter, viz.,

$$q = \int_{\xi}^{\tau_{\infty}} q^{N+1} d\tau / \int_{\xi_{0}}^{\tau_{\infty}} q^{N} \mathcal{R}(\xi, \tau) d\tau . \qquad 9.4$$

Hence the integral equation 9.3 may be written in the form

$$q = \left(\frac{1}{N+2} \right) \int_{\xi}^{\xi_{0}} \int_{z_{0}}^{N+1} dz \left\{ \frac{\int_{\xi}^{q} R(\xi, \tau) d\tau}{\int_{\xi_{0}}^{\xi_{0}} R(\xi, \tau) d\tau} - \frac{\int_{\xi}^{\xi_{0}} R(\xi, \tau) d\tau}{\int_{\xi_{0}}^{\xi_{0}} R(\xi, \tau) d\tau} \right\}$$

$$9.5$$

which does not contain the eigenvalue parameter and includes both boundary conditions.

1 Let us write 9.5 more concisely as

$$q = I(q, \xi, \tau; N)$$
 9.0

In fact, of course, the right hand side of 9.5 or 9.6 is not a function of N at all. Again, on the right of 9.5 or 9.6 the quantities g and g occur only inside integrals which one may assume not to be too sensitive if instead of g and g approximate values of these are substituted. Thus the method of successive approximations is contained in the equations 9.1, 9.2, and

The method is clearly justified if the $g^{(\vee)}$ and $g^{(\vee)}$ form convergent sequences.

The most 'natural' values for N which suggest themselves are N=-1 and N=0 which amount to integration of 7.25 at sight. The choice of the lowest approximation $g^{(0)}$ will be discussed in the following section.

10. DISCUSSION: CHOICE OF LOWEST APPROXIMATION

The solution of the flame equations by the method of successive approximations depends on the choice of a suitable recurrence relation based on 9.3, like 9.7, and on the choice of a suitable lowest approximation $g_{-}^{(o)}$.

The exponent N. As to the first problem, once relation 9.7 is adopted, the following comments on the choice of the exponent are relevant:

N = -/. This case follows by dividing 7.25 by q and integrating; it has been employed in the first order reaction problem of Part I. Advantage: The second ratio on the right of 9.5 is the same for any particular τ at any stage of the operation 9.7. Disadvantages: a) expressions of the form 0/0 occur in the first ratio and these have to be evaluated separately, b) for an unsuitable lowest approximation a supposed $q^{(v+1)}$ may become negative, which entrains an infinite integrand in the succeeding stage - the method breaks down.

N=0. This case follows by integrating 7.25 at sight.

Advantages: a) no ratios of the form 0/0 occur, b) for $\delta = 1$ the first ratio on the right of 9.5 is the same for any particular τ at all stages of the operation 9.7. Disadvantage: for an unsuitable first approximation a supposed $q^{(\lambda, \omega)}$ may become imaginary:- the method breaks down.

N = 1. For an unsuitable first approximation a supposed $q^{(3+1)}$ may become negative, and succeeding $q^{(3)}$ at the same \overline{v} remain negative - the method breaks down.

 $N = \frac{1}{2}$. At first sight none of the more obvious possibilities of a direct break-down of the method, of the kind just described, seem to arise in this case.

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Lowest approximation. It remains to choose a lowest approximation $g^{(o)}$ for the operations 9.7. We consider in detail the case $d^{(i)} = 1$ so that $g^{(i)}$ is a solution of

$$g\left(1-\frac{dq}{d\tau}\right)=q\mathcal{R}_{o}(\tau).$$

It is desirable that the lowest approximation should already possess as many properties as possible of the actual solution; the properties of which follow from 10.1 without further quantitative knowledge of R.(T) are (cf. 8.7-8.11), with increasing T,

- 1) Zero at $\tau = \tau_0$
- 2) Gradient unity at $T = T_0$
 - 3) Maximum occurs on 9 R. (t)
- 2 4) Zero at τ = τ...
- Minimum occurs on $q \mathcal{R}_{o}(\tau)$
 - 6) Gradient unity at $\tau = \tau_{\infty}^*$
 - 7) Further zero at $\tau = t = + \sigma$ (say, where σ is small and positive)
 - 8) Gradient infinite at $\tau = \tau_{\infty}^* + \sigma$ (curve convex to increasing τ)
 - 9) Spiral around T = T*

Since 9 is not known, 3) and 5) are unsuitable for inclusion in any first approximation; similarly, 9) is unsuitable. The remaining conditions cannot be catered for by a polynomial but they are embodied in the following algebraic curve

$$q^{(o)}(\tau) = \frac{1}{(\tau_{eo} - \tau_{o})\sqrt{\tau_{eo}^* + \sigma - \tau_{o}^*}} (\tau - \tau_{o})(\tau_{eo} - \tau)\sqrt{(\tau_{eo}^* + \sigma) - \tau'}, \quad 10.2$$

where o is determined so that

$$\left[\frac{d g^{(0)}(\tau)}{d \tau} \right]_{\tau = \tau_{\infty}^{\#}} = 1 ,$$
 10.3

and one finds that of must be a solution of

$$\frac{16\left(\frac{\sigma}{T_{\infty}^{\#}-T_{\infty}}\right)^{2}-4\left\{\left(\frac{T_{\infty}^{\#}-T_{0}}{T_{\infty}^{\#}-T_{0}}\right)^{2}-\left(\frac{T_{\infty}^{\#}-T_{0}}{T_{\infty}^{\#}-T_{\infty}}\right)+2\right\}\left(\frac{\sigma}{T_{\infty}^{\#}-T_{\infty}}\right)+\left(\frac{T_{\infty}^{\#}-T_{0}}{T_{\infty}^{\#}-T_{0}}\right)=0\ 10.4$$
See quift 13, p.45

Discussion and results. 1. For $\delta = 1$ formula 9.7 reduces

$$g^{(i)+j)} = I(g^{(i)}, \tau; N)$$
 10.5

We took $g^{(o)}$ as in 10.2 and N=0, and performed the operation 10.5 up to $\gamma=10$. Result: The bulk of the $g^{(\gamma)}$ converge; near T_{∞} they diverge, and at the stage $\gamma=10$ the method breaks downsthe integrations were performed by the trapezoidal rule and the last interval adjoining T_{∞} was about $(T_{\infty}-T_{o})/400$; the divergence was oscillatory about fairly definite 'mean' values. When these values were substituted on the right of 10.5 they very nearly reproduced themselves on the left. This suggested use of the formula

$$q^{(\nu+1)} = I\left(\frac{q^{(\nu)}+q^{(\nu-1)}}{2}, \tau; N\right)$$
, 10.6

instead of 10.5, from which we finally obtained 'output' q 's agreeing with the 'input' q 's to any required number of significant digits.

- 2. For $\delta = \frac{3}{4}$ we took $g^{(0)} = g_{\delta=1}$, N = 0, and used a corresponding procedure.
 - 3. Similarly, for $\frac{\delta = 1/2}{2}$, where we started with $g^{(0)} = g_{\beta = 1/2}$
- 4. The attempt of solving the case $\delta = 0$ in a similar manner leads to an immediate break-down of the method when N = 0. We obtained a solution as follows: Extrapolation from $q_{\delta=1}, q_{\delta=3/4}, q_{\delta=2/4}$ gives an approximation to q; this value is used to calculate a parabolic approximation to q near τ_{∞} ; the latter is combined with an approximation to q, extrapolated from $q_{\delta=1}, q_{\delta=3/4}, q_{\delta=2/4}, q_{\delta=$

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We have thus found solutions for the cases $\delta = 1$, $\frac{3}{4}$, $\frac{7}{2}$, 0 which satisfy the flame equations: this is all that is required for practical purposes but the procedure is mathematically dis-See tables 6 -17. tasteful.

Supposing the arbitrary choice of N=0 to be at fault, we have next tried N=/ for the case d=/ with 10.2 as lowest approximation and rigorous application of formula 9.7 or 10.5. Convergence resulted everywhere and for the particular example considered the method thus appears thoroughly satisfactory if one takes

(It may be remarked that the values for 9 8=1. obtained by the two different methods differ by about one per cent - this discrepancy is ascribed solely to the inaccuracy of trapezoidal integration since the integrands involved differ considerably.

g to any required number of significant digits.

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11. ALTERNATIVE METHOD WHEN $d' \neq 1$.

In this section only we adopt the following notation:

$$\mathcal{E} = / - \delta$$
 , 11.1

$$9_0 = 9_0 = 1$$
 , 11.2

$$g_{0} = g_{0} = g_{0$$

$$5. = \int \frac{\tau_{j}}{g_{o}} d\tau \qquad 11.4$$

In order to solve equations 7.19, 7.21,

$$g\left(i - \frac{dg}{d\xi}\right) = g\left(\mathcal{R}_0 + \mathcal{R}_1 \xi + \mathcal{R}_2 \xi^2\right), \quad 11.5$$

$$(i-\varepsilon)g\frac{d\xi}{d\varepsilon}-\xi=-\varepsilon\ell g, \qquad 11.6$$

we assume the expansions

$$q = \frac{q_0}{1 + \epsilon q_1 + \epsilon^2 q_2 + \cdots}$$
, 11.7

$$g = g_0 + \epsilon g_1 + \epsilon^2 g_2 + \cdots, \quad 11.8$$

$$\xi = \frac{\epsilon \xi}{11.9} + \frac{\epsilon^2 \xi_2 + \cdots}{11.9}$$

where the suffixed quantities are independent of ε (i.e. of δ), substitute them into 11.5, 11.6, and equate coefficients of powers of ε . The solution for the case $\varepsilon = 0$ is supposed known; we abbreviate

$$\chi_1 = \frac{q_1}{q_2}$$
, $\chi_2 = \frac{q_2}{q_2}$, ...; 11.10

the resulting <u>linear</u> equations are now easily integrated in the following order:

$$\xi_{1} = \mathcal{R} e^{\xi_{0}} \int_{c}^{c} e^{-\xi_{0}} d\tau , \qquad 11.11$$

$$g_{1} = g_{0} \frac{1}{g_{0}} e^{\xi_{0}} \left[-g_{1} \int_{c}^{\tau_{0}} e^{-\xi_{0}} \mathcal{R}_{0} d\tau + \int_{c}^{\tau_{0}} e^{-\xi_{0}} \mathcal{R}_{1} \xi_{1} d\tau \right], 11.12$$

where

$$q_{i} = \int_{\tau}^{\tau_{o}} e^{-S_{o}} \mathcal{E}_{i} \, \xi_{i} \, dx / \int_{\tau_{o}}^{\tau_{o}} e^{-S_{o}} \, \chi_{o} \, d\tau \quad . 11.13$$

1

11.18

$$\xi_{2} = \xi_{1} - e^{\xi_{2}} \int_{c}^{\tau_{2}} e^{-\xi_{1}} (1 - \chi_{1}) \frac{\xi_{1}}{g_{0}} d\tau$$

$$q_{2} = q_{0} \frac{1}{g_{0}} e^{\xi_{0}} \left(- q_{2} \int_{c}^{\tau_{2}} e^{-\xi_{0}} \mathcal{R}_{0} d\tau \right)$$

$$+ \int_{c}^{\tau_{2}} e^{\xi_{0}} \left[(q_{1}^{2} + q_{1}\chi_{1}^{2} + \chi_{1}^{2}) \mathcal{R}_{0} + \mathcal{R}_{1}^{2} \left\{ \xi_{2} - (q_{1} + \chi_{1}^{2}) \xi_{1}^{2} \right\} + \mathcal{R}_{2}^{2} \xi_{1}^{2} d\tau \right] 11.15$$

where

$$q_{2} = \frac{\int_{c}^{t_{a}} S_{a} \left[(q_{1}^{2} + q_{1} f_{1} + g_{1}^{2}) g_{0}^{2} + g_{1} f_{1}^{2} + g_{1}^{2} g_{1}^{2} + g_{1}^{2} g_{1}^{2} + g_{1}^{2} g_{1}^{2} g_{1}^{2} + g_{1}^{2} g_{1}^{2} g_{1}^{2} g_{1}^{2} + g_{1}^{2} g_{1}^{2} g_{1}^{2} g_{1}^{2} g_{1}^{2} + g_{1}^{2} g_{$$

$$\xi_{3} = \xi_{2} - e^{\xi_{3}} \int_{c}^{\xi_{3}} e^{-\xi_{3}} \left\{ (1 - \xi_{1}^{2}) \frac{\xi_{2}}{g_{2}} + (\xi_{1}^{2} - \xi_{2}^{2}) \frac{\xi_{1}}{g_{3}} \right\} d\tau$$
11.17

$$g_{3} = q_{0} + \frac{1}{q_{1}} e^{\xi_{0}} \left(-q_{3} \int_{\xi}^{\xi_{0}} e^{-\xi_{0}} \mathcal{R}_{0} dt \right)$$

$$+ \int_{\xi}^{\xi_{0}} \left[\left\{ q_{1} (2q_{2} - q_{1}^{2}) + \delta_{3} (q_{1} + \delta_{1}^{2}) + \delta_{1} (q_{2} + \delta_{2}^{2}) - \delta_{1} (q_{1}^{2} + q_{1}^{2} r_{1} + r_{1}^{2}) \right\} \mathcal{R}_{0} \right]$$

$$+ \mathcal{R}_{1} \left[\left\{ q_{1}^{2} + \delta_{1} (q_{1} + \delta_{1}^{2}) - (q_{2} + \delta_{2}^{2}) \right\} \right] dt$$

$$+ \mathcal{R}_{2} \left\{ 2\xi_{1} \xi_{2} - (q_{1} + \delta_{1}^{2}) \xi_{1}^{2} \right\} dt$$

where

$$\int_{\zeta_{o}}^{\tau_{o}} (\text{same integrand as in second integral of 11.18}) d\tau$$

$$\int_{\zeta_{o}}^{\tau_{o}} (\text{same integrand as in second integral of 11.18}) d\tau$$

$$\int_{\zeta_{o}}^{\tau_{o}} (\text{same integrand as in second integral of 11.18}) d\tau$$

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$$\int_{\zeta_{o}}^{\tau_{o}} (\text{same integrand as in second integral of 11.18}) d\tau$$

etc. See graph 22, p. 53

12. NEGLECT OF BACK REACTION; VARIATION OF HOT BOUNDARY TEMPERATURE

Neglect of the back reaction. It was desirable to show that the method is unaffected, and the results little changed, if the back-reaction is neglected. In this case, if one considers only $\delta = 1$, cf. A.4,

$$\mathcal{R}_{o}(\tau) = (\chi^{*})^{2} \varphi(\tau)$$

$$= \left(\frac{\tau_{oo} - \tau}{\tau_{oo} - \tau_{o}}\right)^{2} \varphi(\tau)$$
12.1

Here τ_{∞} and $\tau_{\infty}^{\#}$ coincide, and $x_{\infty} = 0$. As lowest approximation one takes

$$g^{(0)} = \frac{1}{(\overline{\tau_{\infty} - \tau_{0}})^{2}} (\overline{\tau} - \overline{\tau_{0}}) (\overline{\tau_{\infty} - \tau})^{2}. \quad 12.3$$

One finds the expected results, but very near τ_{∞} , when 10.5 is used there is again no convergence and formula 10.6 has to be applied; use of $N=\frac{1}{2}$, $\frac{3}{2}$, give consistent results. Cf. graph 24.

Variation of the hot boundary temperature. It is also of interest to investigate how the eigenvalue parameter q changes with τ_{∞} when τ_{∞} is kept constant. The procedure outlined just above was thus repeated for different τ_{∞} with formulae 12.2 and 12.3. The results are shown in graphs 23 and 24.

APPENDIX

Simple chain reaction flame. Let us consider an idealized flame based on the reactions

$$A \rightleftharpoons B$$

$$A + B \implies B + C$$
 / A.2

and let we suppose that to a first approximation component $\, \beta \,$ is in equilibrium with $\, A \,$, so that

$$\chi_{B} = \varphi(\tau) \chi_{A} . \qquad A.3$$

The rate of decrease of component A (which we have roughly referred to as the reaction rate) may be assumed as proportional to

$$x_{B}x_{A} - x_{B}(1-x_{A}-x_{B}) \Phi(\tau) , \qquad A.4$$

that is,

$$\chi_{A} \varphi(\tau) \left[\chi_{A} - \left\{ 1 - \chi_{A} - \chi_{A} \varphi(\tau) \right\} \Phi(\tau) \right].$$
 A.5

Dropping the suffix A, we see that the problem is equivalent to that of a unimolecular reaction of the type already considered*, with the total reaction rate of the fuel component of the second order and proportional to

 $R(X,\tau) = \chi \left(\chi \left[\varphi(\tau) + \varphi(\tau) \Phi(\tau) + \left\{ \varphi(\tau) \right\}^2 \Phi(\tau) \right] - \varphi(\tau) \Phi(\tau) \right). A.6$ If at the hot boundary temperature τ_{∞} a fraction X_{∞} of the fuel is left,

$$\chi_{\omega} = \frac{\Phi(\tau_{\omega})}{1 + \Phi(\tau_{\omega}) + \varphi(\tau_{\omega})\Phi(\tau_{\omega})} \qquad A.7$$

We note that X is a factor of the total reaction rate R(X, z),

$$R(0,\tau)=0$$

Thus, in terms of a unimolecular reaction one could say that the fuel acts at the same time as a catalyst whose presence is indispensable.

^{*} This is not gun to true: there is an additional them is the energy equ. 1.3 The full ABC problem will be considered in a forthcoming report.

Particular example.

$$\Phi(z) = \varphi(z).$$

A.9

In the original formulation of the problem $\varphi(z)$ was taken to be equal to e-1/t ; in the present treatment we have put

A. 10

and chosen the constant K so as to get simple expressions for and the linear function x^* of 7.7.(or 7.10). Thus with

A. 11

A.12

A. 13

so that, cf. 7.8, 6 = 5 , and by A.7,

$$\chi_{\infty} = \frac{1}{100} = \frac{\kappa e^{-1/\tau_{\infty}}}{1 + \kappa e^{-1/\tau_{\infty}} + (\kappa e^{-1/\tau_{\infty}})^2} A_1 14$$

which gives

A.15

On comparison of A.6 and 7.15 one finds

$$\mathcal{R}_{z}(t) = \varphi(t) + \left\{\varphi(t)\right\}^{2} + \left\{\varphi(t)\right\}^{3}$$

A. 16

$$\mathcal{R}_{1}(\tau) = 2x^{*}\mathcal{R}_{2}(\tau) - \{\varphi(\tau)\}^{2}$$

A. 17

and $\mathcal{R}_{a}(\tau)$ is given by 8.3.

to ricular example. We take

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Without many constructive discussions with Professor

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is the average locardition of the problem 912) was taken to be

- J. O. Hirschfelder, Professor C. F. Curtiss, and Dr.
- E. S. Campbell, the author would have found nimself in a succession of blind alleys. If the present method should eventually prove to be a satisfactory one for a mathematical description of flames, it will in no small measure have been based on their experience, so readily shared.

The following members of the staff of the Naval Research Laboratory have contributed to the production of this report, and their assistance is gratefully acknowledged: Mrs. L. Brittenham, Mrs. N. Lowry, Mrs. P. Reese, Mrs. M. Schanzenbach. and Mrs. E. Silversmith.

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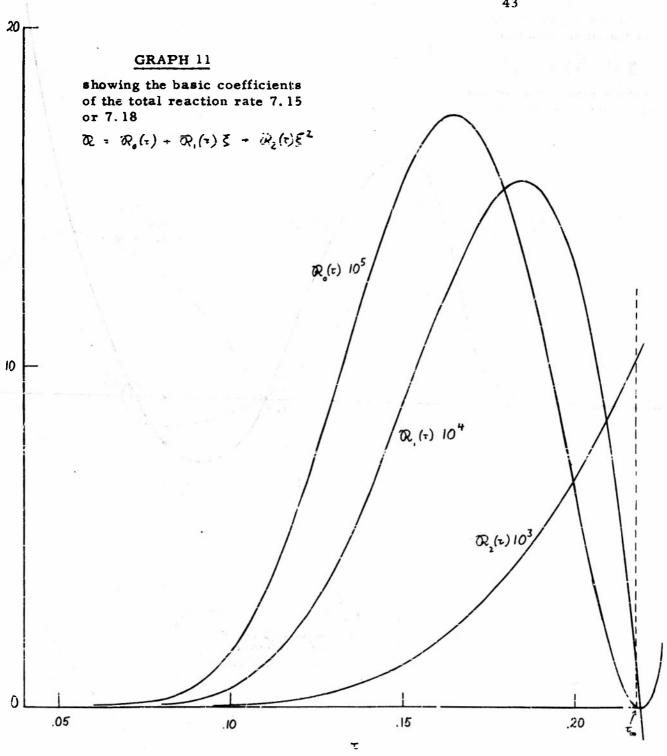
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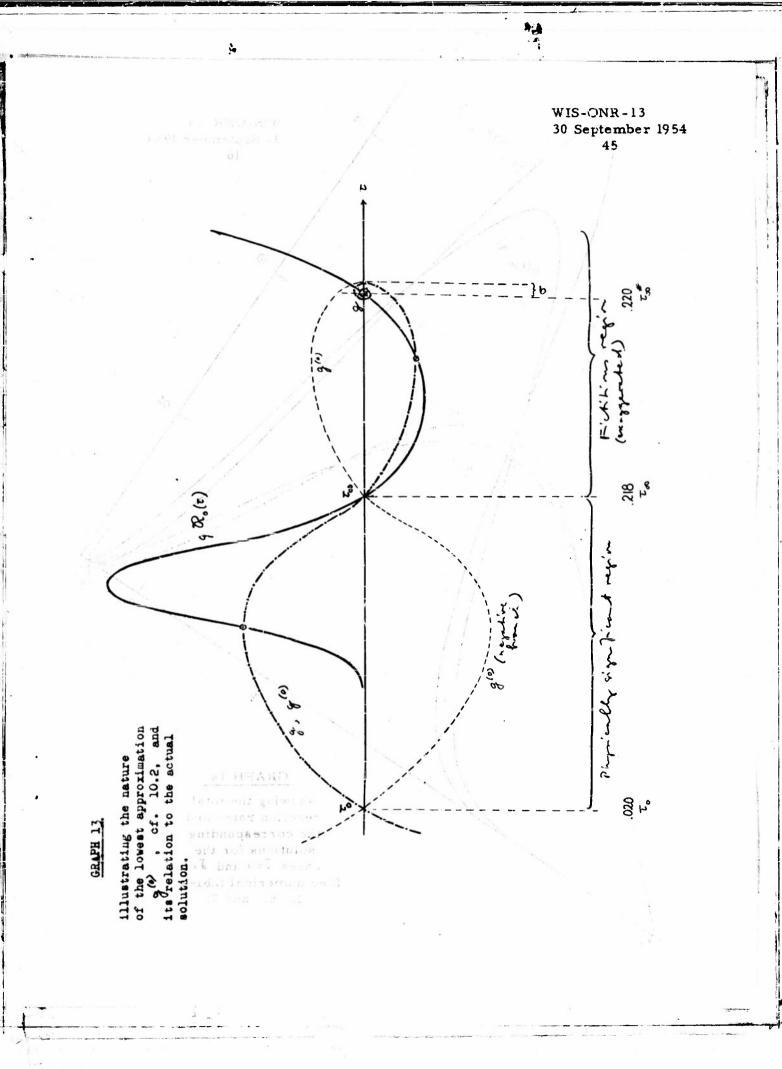
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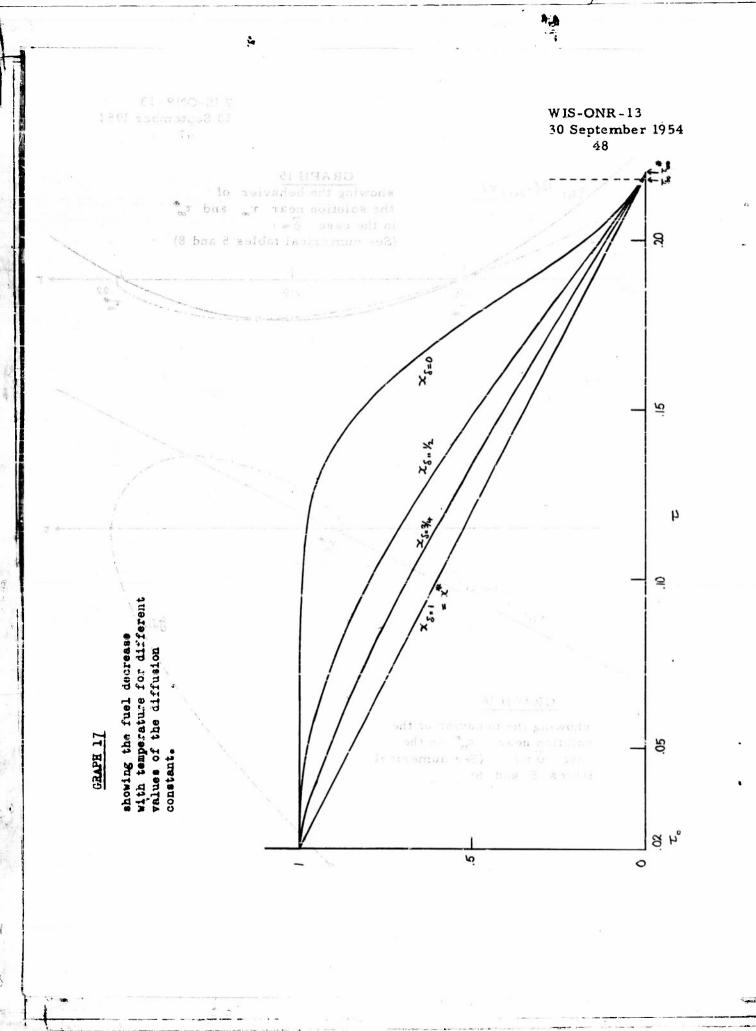
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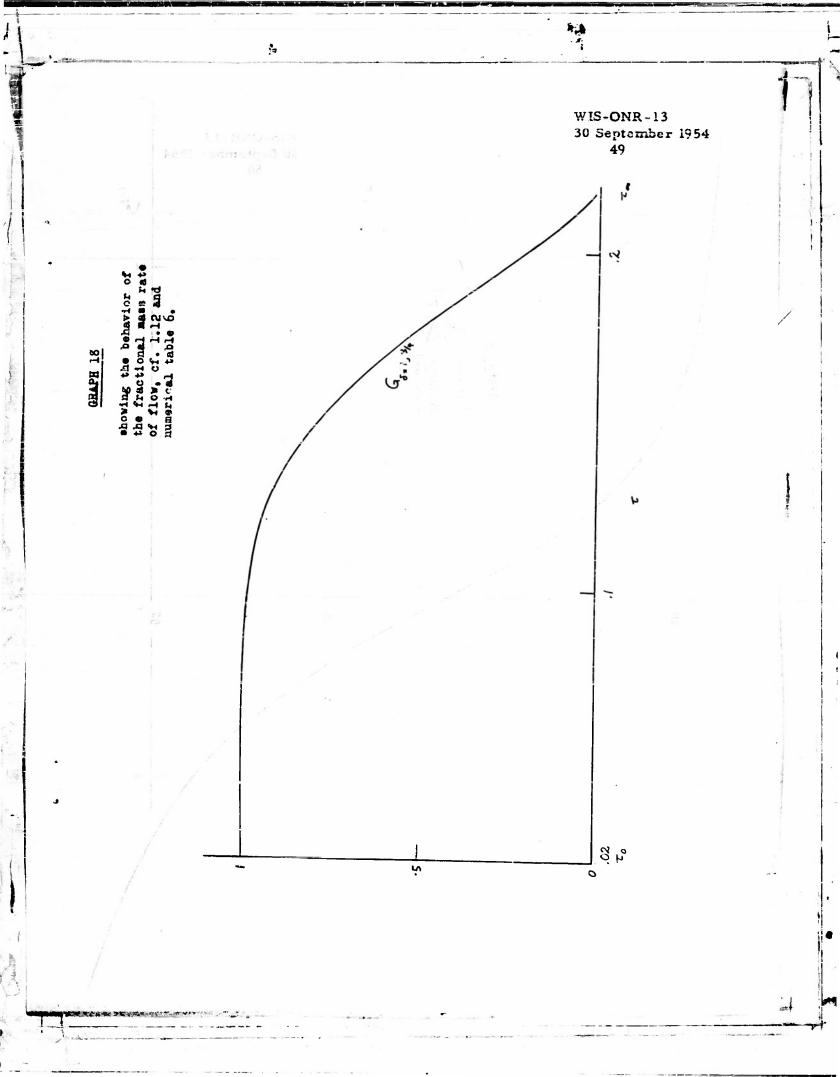
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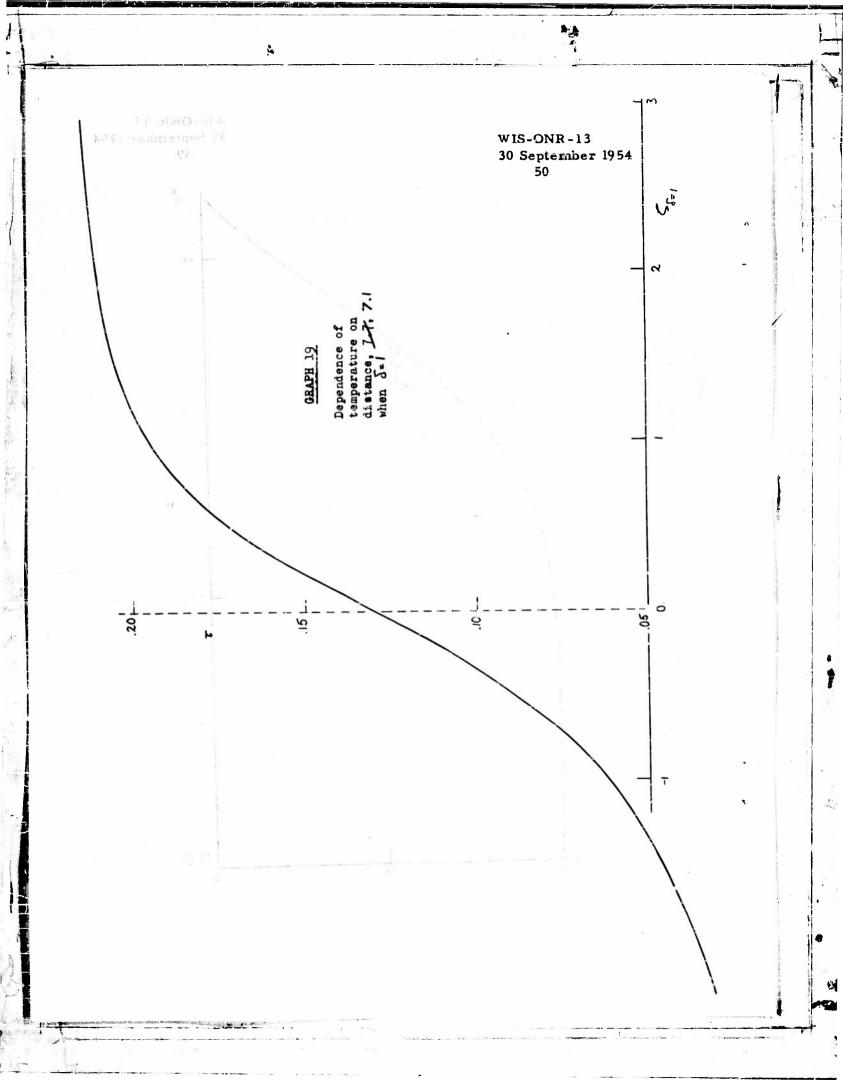


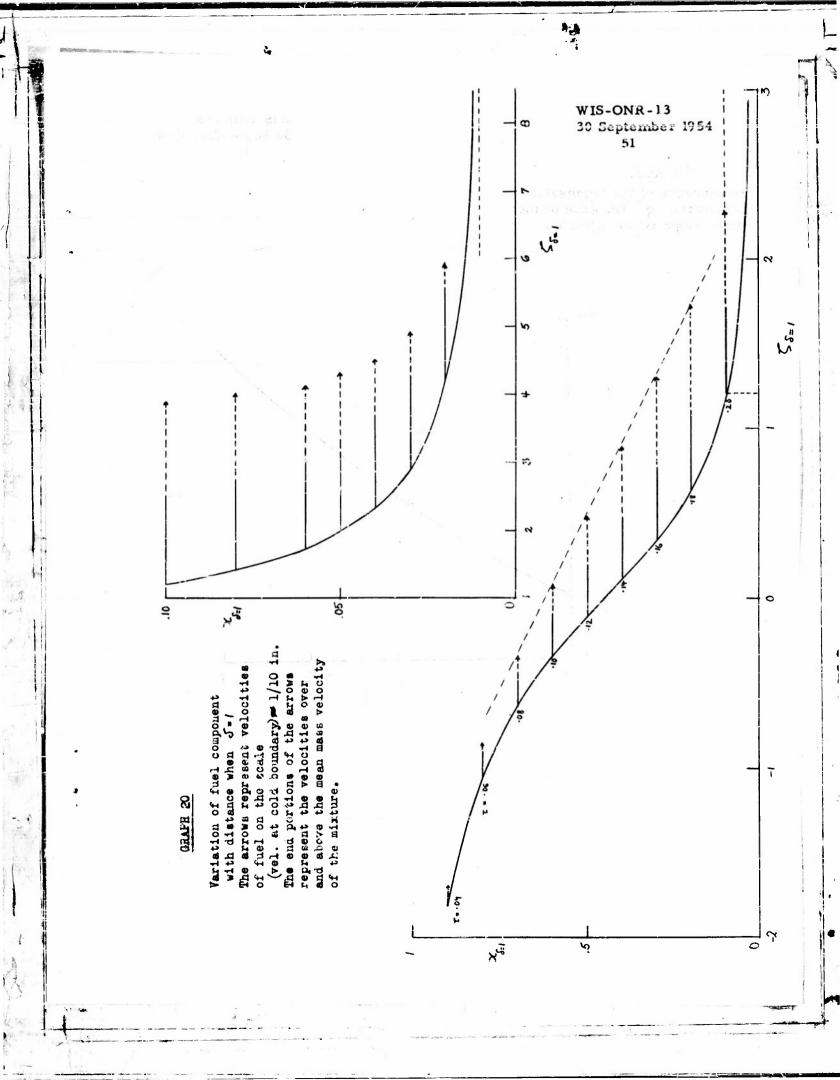


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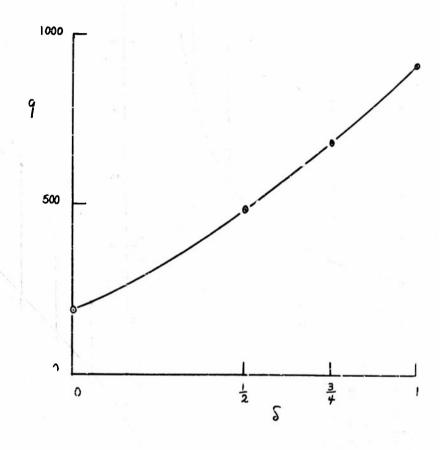






GRAPH 21

Dependence of the eigenvalue parameter q (inverse of the flame velocity) on diffusion



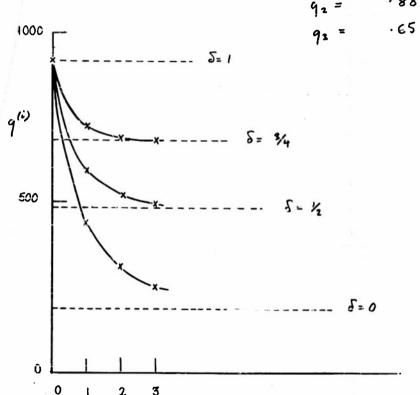
GRAPH 22

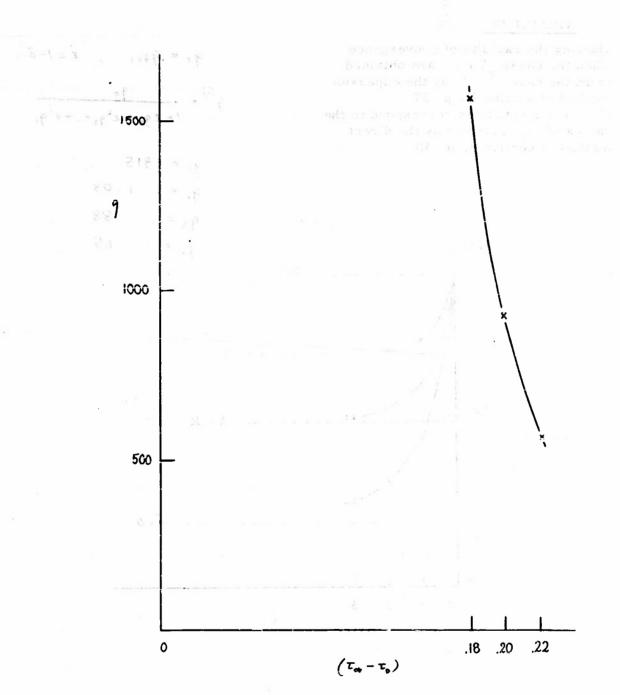
showing the rapidity of convergence when the cases $S \neq I$ are obtained from the case S = I by the expansion method of scation 11, p. 37 (The horizontal lines correspond to the values of q obtained by the direct method of section 9, p. 31)

$$q_0 = \hat{q}_{\delta = 1}, \quad \varepsilon = 1 - \delta$$

$$q_0 = \frac{q_0}{1 + \varepsilon q_1 + \varepsilon^2 q_2 + \dots + \varepsilon^2 q_i}$$

$$q_0 = 913$$
 $q_1 = 1.08$
 $q_2 = .88$
 $q_3 = .65$



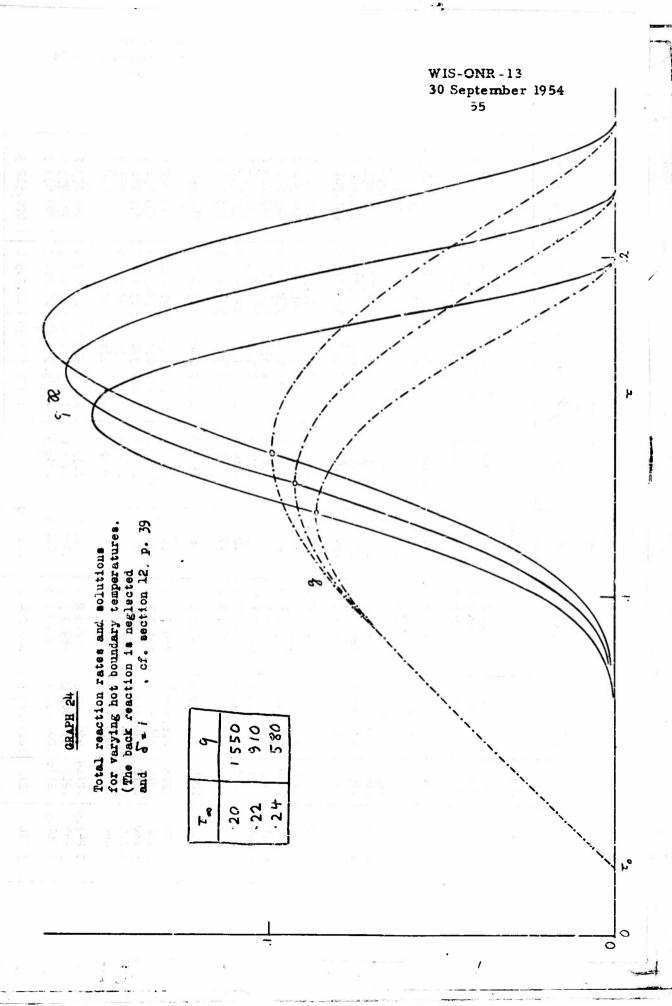


GRAPH 23

Dependence of the parameter q on the hot boundary temperature. (The back reaction is neglected, $\delta = 1$, and the cold boundary temperature is kept constant; Cf. section 12, p. 39)

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Q (c) × 102		.000 0 .005 8 .369 9	4.504 7 11.181 7 23.854 2 45.295 5 78.491 5 126.426 4	277 405 6 328.342 0 385.041 4 447.700 8 516.490 6 591.556 1 673.017 2	742.856 9	816.891.6 855.491.9 895.151.8 935.873.9 977.660.2	988.273 2 998.953 0 1 009.699 3	1 020.512 3
R, (E) x 105		.000 5 2 600. 7 713.	5.405 4 12.298 5 23.848 5 40.745 5 62.731 7 88.339 0	137.937 5 146.683 0 152.545 11 154.708 7 152.306 9 141.430 6 130.134 2	6 614.811	91.461 6 78.354 2 63.740 8 47.555 5 29.732 4	20.185 9 20.185 9 15.250 3	10.205 1
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R, CE) x 105	ı	.000 0 .003 7 .181 2	1.621 6 3.383 7 5.960 7 9.163 1 12.534 0 15.431 4	17.146 5 16.381 3 15.107 4 13.363 2 11.225 0 8.810 8 6.283 3	4.319 3	2.546 9 1.779 0 1.117 4 584 4 203 6	.135 1 .078 0 .032 9	0 0
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TABLE 8

ACCOUNTS TO THE TOTAL PORT OF THE PARTY OF T		TL 05 (A) L	
\$6555	J s=1	dgs.,	Parabolic approximation
217 .217 2 .217 4 .217 6 .217 8	.000 460 .000 351 .000 253 .000 160 .000 076		.000 475 .000 358 .000 255 .000 161 .000 076
.218	0	358 0	0
.218 2 .218 4 .218 6 .218 8 .219	000 066 000 124 000 171 000 207 000 229		.000 067 .000 125 .000 174 .000 215
.219 2 .219 4 .219 6 .219 8	000 238 M 000 230 000 203 000 145	1	.000 268 .000 281 .000 286 M .000 281

(A= - T/2	5 = r-7/2
6006	1/r-1/2
- 90° - 60° - 45° - 15° - 30° - 15° - 15° - 15° - 15° - 180° - 180° - 180° - 180° - 240° - 270°	1 .701 0 .647 6 .628 5 .632 7 .642 8 .602 9 .463 0 .411 9 .195 8 .099 7 .045 2 .031 8 .029 5 .020 9 .016 9

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